mercaptoacetaldehyde

Other names: Acetaldehyde, mercapto-
Inchi: InChI=1S/C2H4OS/c3-1-2-4/h1,4H,2H2
InchiKey: FLJWVVUJGVNXMZ-UHFFFAOYSA-N
Formula: C2H4OS
SMILES: O=CCS
Mol. weight [g/mol]: 76.12
CAS: 4124-63-4

Physical Properties

Property code	Value	Unit	Source
gf	-104.17	kJ/mol	Joback Method
hf	-131.71	kJ/mol	Joback Method
hfus	7.27	kJ/mol	Joback Method
hvap	33.50	kJ/mol	Joback Method
ie	10.00 ± 0.02	eV	NIST Webbook
log10ws	-0.01		Crippen Method
logp	0.115		Crippen Method
mcvol	56.960	ml/mol	McGowan Method
pc	6180.53	kPa	Joback Method
rinpol	658.00		NIST Webbook
rinpol	660.00		NIST Webbook
rinpol	658.00		NIST Webbook
rinpol	660.00		NIST Webbook
tb	356.68	K	Joback Method
tc	558.87	K	Joback Method
tf	190.76	K	Joback Method
vc	0.218	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	85.09	J/mol×K	356.68	Joback Method
cpg	89.38	J/mol×K	390.38	Joback Method
cpg	93.48	J/mol×K	424.08	Joback Method

cpg	97.41	J/mol×K	457.78	Joback Method
cpg	101.15	J/mol×K	491.47	Joback Method
cpg	104.73	J/mol×K	525.17	Joback Method
cpg	108.13	J/mol×K	558.87	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4124634&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume